# Chapter 1 : Wavefunctions

## 1-28-19

Classical Mechanics : $\vec{F} = \frac{d\vec{p}}{dt} = m\frac{d\vec{v}}{dt} + \vec{v}\frac{d\vec{m}}{dt}$    Vector : $\vec{r}(0), \vec{v}(0)$

$\vec{F} = -\vec{\nabla} V$ for conservative forces : $\boxed{\text{Deterministic}}$

Quantum Mechanics : $\Psi(\vec{r},t) \to$ Scalar    S.E : $i\hbar \frac{\partial \Psi}{\partial t} = \hat{H}\Psi \to \Psi$

SE solves for $\Psi$ of a quantum, spinless, non-relativistic system

Big deal ? : Get energies $\to$ bound $\to$ discrete
$\to$ free $\to$ continuous

1D SE : $i\hbar \frac{\partial \Psi}{\partial t} = \frac{-\hbar^2}{2m}\frac{\partial^2 \Psi}{\partial x^2} + \hat{V}\Psi$ : $\hbar = \frac{h}{2\pi} = 1.054572 \times 10^{-34}$ J·S

1D Time Independent SE : $\hat{H}\Psi = E\Psi$

Quantum Mechanics is statistical in nature

Steps :
1) Solve SE for a given potential $\to$ you get $\Psi$
2) Given $\Psi$ normalize it $\to \int \Psi\Psi^* dx = 1$
3) To find probability that particle will be found in $x \in [a,b] \to \int_a^b |\Psi|^2 dx$
4) To measure a physical quantity like $E, x, P_x$, etc
apply the corresponding operator $\hat{Q}$ to $\Psi$ if $\hat{Q}\Psi = q\Psi$, then $q$ is value
if not $q\Psi$ can't measure

$\hat{V} = 0$ Free particle , $\Psi = e^{i(kx-\omega t)}$

$$\Psi\Psi^* = e^{i(kx-\omega t)}e^{-i(kx-\omega t)} = 1 \to \int_{-\infty}^{\infty} 1\, dx = 2\cdot\infty$$

$$i\hbar\frac{\partial \Psi}{\partial t} = \frac{-\hbar^2}{2m}\frac{\partial^2 \Psi}{\partial x^2} : i\hbar\frac{\partial \Psi}{\partial t} = i\hbar(-i\omega)\Psi = \hbar\omega\Psi : -\hbar^2 \quad i\hbar\frac{\partial}{\partial t} \to \hat{E}\Psi = \hbar\omega\cdot\Psi$$

$$-\frac{\hbar^2}{2m}\cdot\frac{\partial^2 \Psi}{\partial x^2} = \frac{\hbar^2 k^2}{2m}\Psi : 1\cdot\frac{\partial \Psi}{\partial x} = ik\Psi \quad 2\; ik\frac{\partial \Psi}{\partial x} = (ik)^2\Psi$$

Free particle    $\hat{E}$

$E = \hbar\omega \to i\hbar\frac{\partial \Psi}{\partial t}$

$KE = \frac{\hbar^2 k^2}{2m} \to -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$

$P = \hbar k$

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| | Bound | Free |
|---|---|---|
| Probabilities $\rightarrow$ | Discrete, | Continuous |
| | Onevalue, | Range of values |

| j $\rightarrow$ Value | | N(j) |
|---|---|---|
| 14 | $\rightarrow$ | 1 |
| 15 | $\rightarrow$ | 1 |
| 16 | $\rightarrow$ | 3 |
| 22 | $\rightarrow$ | 2 |
| 24 | $\rightarrow$ | 2 |
| 25 | $\rightarrow$ | 5 |

$N = \sum_{j=0}^{\infty} N(j) = 14$

$P(j) = \frac{N(j)}{N}$, $\sum_{j=0}^{\infty} P(j) = 1$, $\langle j \rangle = \sum j \cdot P(j)$ = Expectation Value

$\langle j^2 \rangle = \sum \frac{j^2 N(j)^2}{N} = \sum j^2 P(j^2)$

$\langle f(j) \rangle = \sum F(j) P(j)$

$\langle j^2 \rangle \neq \langle j \rangle^2$

Spread

$\Delta j = j - \langle j \rangle$

$\langle \Delta j \rangle = \sum (j - \langle j \rangle) P(j) = \sum j (P(j)) - \sum \langle j \rangle P(j) = \langle j \rangle - \langle j \rangle \sum P(j) = 0$

$\sqrt{\sigma^2}$ - Characterizes width

$\langle (\Delta j)^2 \rangle$, $\langle (\Delta j)^2 \rangle \langle j^2 - 2j\langle j \rangle + \langle j \rangle^2 \rangle = \langle j^2 \rangle - \langle 2j \langle j \rangle \rangle + \langle \langle j \rangle^2 \rangle$

$= \langle j^2 \rangle - 2\langle j \rangle \langle j \rangle + \langle j \rangle^2$

$= \langle j^2 \rangle - 2\langle j \rangle^2 + \langle j \rangle^2$

$= \langle j^2 \rangle - \langle j \rangle^2$

$\sigma = \sqrt{\langle j^2 \rangle - \langle j \rangle^2}$ $\qquad \sigma_x \sigma_{p_x} \geq \frac{\hbar}{2}$

$\Psi = \begin{cases} A\frac{x}{a} & 0 \leq x \leq a \\ A\frac{(b-x)}{(b-a)} & a \leq x \leq b \end{cases} \rightarrow \int_0^a A^2 \cdot \frac{x^2}{a^2} + \int_a^b A^2 \frac{(b-x)^2}{(b-a)^2} dx = 1$

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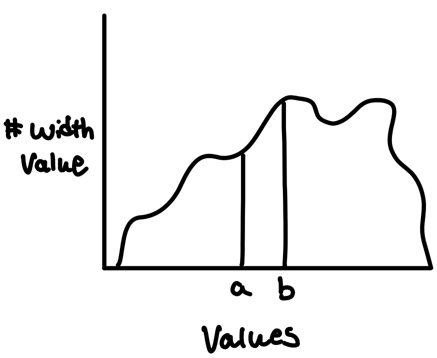
| j | N(j) | P(j) |
|---|---|---|
| 1 | 1 | 1/6 |
| 2 | 1 | 1/6 |
| 3 | 1 | 1/6 |
| 4 | 1 | 1/6 |
| 5 | 1 | 1/6 |
| 6 | 1 | 1/6 |

$\langle j \rangle = \frac{1}{6} + \frac{2}{6} + \frac{3}{6} + \frac{4}{6} + \frac{5}{6} + \frac{6}{6} = \frac{7}{2}$

$\langle j \rangle^2 = \frac{49}{4}$, $\langle j^2 \rangle = \frac{1}{6}(1+4+9+16+25+36) = \frac{91}{6}$

$\sigma = \sqrt{\frac{91}{6} - \frac{49}{4}} \cong 1.707$




Probability density

$P \in [x, x+dx] = \rho(x) dx$

$\Psi$ Wavefunction $\rightarrow \rho(x) = \Psi \Psi^*$

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## Continuous Variables

$P \in [x, x+dx] = \rho(x)\,dx$ $\qquad \rho(x) = \Psi \cdot \Psi^*$

Probability density

careful $\rho(x) =$ give but if they give $\Psi = \Psi\Psi^*$

$\int \rho(x)\,dx = 1$, $\int \Psi \cdot \Psi^*\,dx = 1$, $\langle F(j)\rangle = \sum F(j)P(j)$, $\langle F(j)\rangle = \int \Psi^* f(x)\,\Psi\,dx$

$[0, \pi] \rightarrow PDF = A$

$\int_0^\pi A\,d\theta = 1$, $A\theta\Big|_0^\pi = 1$, $A \cdot \pi = 1$, $A = \frac{1}{\pi} = PDF = \rho(\theta)$


$$\langle \theta \rangle = \int_0^\pi \theta \cdot \frac{1}{\pi}\,d\theta = \frac{\theta^2}{2}\Big|_0^\pi \cdot \frac{1}{\pi} = \frac{\pi^2}{2\pi} \cdot \frac{\pi}{2}$$

$$\langle \theta^2 \rangle = \frac{1}{\pi}\int_0^\pi \theta^2\,d\theta = \frac{\theta^3}{3\pi}\Big|_0^\pi = \frac{\pi^2}{3}$$

## Normalizable : $\Psi \rightarrow 0$ at $\pm\infty$

#1: $\Psi = A e^{-\lambda|x|} e^{-i\omega t}$

#2: $$\int_{-\infty}^{\infty} A^2 e^{-2\lambda|x|}\,dx = 1 \rightarrow A^2 \int_0^\infty e^{-2\lambda x}\,dx = \frac{1}{2} \rightarrow -\frac{A^2}{2\lambda}\left[e^{-2\lambda x}\right]_0^\infty = \frac{1}{2}$$

$$\frac{A^2}{2\lambda}\left[e^{-2\lambda x}\right]_\infty^0 = \frac{1}{2} : \frac{A^2}{\lambda}\left[e^0 - e^{\infty}\right] = 1 : \frac{A^2}{\lambda} = 1 \quad \therefore \quad A = \sqrt{\lambda}$$

$$\Psi(x,t) = \sqrt{\lambda}\, e^{-(\lambda|x| + i\omega t)}$$

Steps:
1.) Get $\Psi$
2.) Normalize $\Psi$
3.) $P \in [a,b] = \int_a^b \Psi\Psi^*\,dx$
4.) $\hat{Q}\Psi_{iff} = q\Psi$

Physical Quantity

value measured

$$\langle x \rangle = \frac{2}{a}\int_0^a x \sin^2\left(\frac{\pi x}{a}\right) dx \rightarrow \frac{1}{a}\int_0^a \left(x - x\cos\left(\frac{2\pi}{a}x\right)\right) dx$$

$$\frac{1}{a}\int_0^a x\,dx - \frac{1}{a}\int_0^a x\cos\left(\frac{2\pi}{a}x\right) dx$$

$u = x$ $\qquad v' = \cos\left(\frac{2\pi}{a}x\right)$

$du = dx$ $\qquad v = \frac{a}{2\pi}\sin\left(\frac{2\pi}{a}x\right)$

$$\frac{1}{a}\left[\frac{x^2}{2} - \left(\frac{ax}{2\pi}\sin\left(\frac{2\pi}{a}x\right)\Big|_0^a - \int_0^a \frac{a}{2\pi}\sin\left(\frac{2\pi}{a}x\right)dx\right)\right] = \frac{1}{a}\left[\frac{a^2}{2} - \left(0 + \left(\frac{a}{2\pi}\right)^2 \cos\left(\frac{2\pi}{a}x\right)\Big|_0^a\right)\right]$$

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$\frac{d\langle x\rangle}{dt} = ?$ , $\int |\Psi(x,t)|^2 = 1$ for all time

$$\frac{d}{dt}\int_{-\infty}^{\infty} |\Psi(x,t)|^2\,dx = \int_{-\infty}^{\infty} \frac{\partial}{\partial t}\cdot \Psi\Psi^*\,dx \quad , \quad \text{Inside} = \dot{\Psi}\Psi^* + \Psi\dot{\Psi}^*$$

$$SE = i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} + V(\Psi) \quad , \quad SE = \dot{\Psi} = \left(-\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} + V(\Psi)\right)\cdot\frac{1}{i\hbar}\frac{i}{i} = \frac{-i}{\hbar}\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(\Psi)\right)$$

$$\dot{\Psi} = \frac{i\hbar}{2m}\Psi'' - \frac{iV(\Psi)}{\hbar} \quad , \quad \dot{\Psi}^* = \frac{-i\hbar\Psi^*}{2m} + \frac{iV(\Psi^*)}{\hbar}$$

$$\frac{\partial}{\partial t}|\Psi|^2 = \dot{\Psi}\Psi^* + \Psi\dot{\Psi}^* \quad , \quad \Psi^*\left[\frac{i\hbar\Psi''}{2m} - \frac{i}{\hbar}V(\Psi)\right] + \Psi\left[\frac{-i\hbar}{2m}(\Psi^*)'' + \frac{i}{\hbar}V(\Psi^*)\right]$$

$$= \frac{i\hbar}{2m}\left[\Psi^*\Psi'' - \Psi(\Psi^*)''\right] = \frac{i\hbar}{2m}\frac{\partial}{\partial x}\left[\Psi^*\Psi' - (\Psi^*)'\Psi\right]$$

$$\frac{d}{dt}\int |\Psi(x,t)|^2\,dx = \frac{i\hbar}{2m}\int_{-\infty}^{\infty}\frac{\partial}{\partial x}\left[\Psi^*\Psi' - (\Psi^*)'\Psi\right]dx = \frac{i\hbar}{2m}\left[\Psi^*\Psi' - (\Psi^*)'\Psi\right]\Big|_{-\infty}^{\infty} = 0$$

rule $\langle\hat{Q}\rangle = \int \Psi^*\hat{Q}\Psi$

$$\frac{d\langle x\rangle}{dt} = \frac{i\hbar}{2m}\int x\frac{\partial}{\partial x}\left[\Psi^*\Psi' - (\Psi^*)'\Psi\right]dx$$

$\int \frac{d}{dt}[uv] = \int[\dot{u}v + u\dot{v}] \longrightarrow uv\Big|_a^b - \int_a^b v\,du = \int_a^b u\,dv$ : Purpose is to switch derivatives

$x = u \qquad dv = \frac{\partial}{\partial x}\left[\Psi^*\Psi' - (\Psi^*)'\Psi\right]dx$

$dx = du$

$\qquad V = \Psi^*\Psi' - (\Psi^*)'\Psi$

$$\frac{d\langle x\rangle}{dt} = \frac{i\hbar}{2m}\cdot\left[\left[x\left(\Psi^*\Psi' - (\Psi^*)'\Psi\right)\right]_{-\infty}^{+\infty} - \int\left(\Psi^*\Psi' - (\Psi^*)'\Psi\right)dx\right]$$

$$\frac{i\hbar}{2m}\int -\left[\Psi^*\Psi' + (\Psi^*)'\Psi\right]dx$$

$$\longrightarrow = \frac{i\hbar}{2m}\cdot\cancel{\Psi^*\Psi\Big|_{-\infty}^{\infty}}^{\,0} - \frac{i\hbar}{2m}\int \Psi^*\frac{\partial\Psi}{\partial x}\,dx$$

$$= \frac{-i\hbar}{m}\int \Psi^*\Psi'\,dx = \frac{-i\hbar}{m}\int \Psi^*\frac{d}{dx}\Psi\,dx = \frac{d\langle x\rangle}{dt}$$

$$-i\hbar\int \Psi^*\frac{d}{dx}\Psi\,dx = m\frac{d\langle x\rangle}{dt} = \langle P\rangle \qquad \boxed{\hat{P}_x = -i\hbar\frac{d}{dx}}$$

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$$\frac{d\langle x\rangle}{dt} = -i\hbar\int \Psi^* \frac{\partial \Psi}{\partial x}\,dx = \frac{\langle \hat{p}\rangle}{m}$$ : Expectation values follow classical mechanics

$$\frac{d\langle p\rangle}{dt} = -\left\langle \frac{\partial V}{\partial x}\right\rangle = \langle p\rangle$$

$$\hat{H} = \hat{T} + \hat{u}$$

$$\frac{1}{2}m\hat{v}^2 = \frac{\hat{p}^2}{2m} \rightarrow \hat{p}^2 = (i\hbar)^2\frac{\partial^2}{\partial x^2} \rightarrow \hat{p} = -i\hbar\frac{\partial}{\partial x} = \frac{\hbar}{i}\frac{\partial}{\partial x}$$

$$\Psi(x) = \sqrt{\frac{2}{a}}\sin\left(\frac{\pi x}{a}\right)$$

$$\hat{p}\Psi = -i\hbar\sqrt{\frac{2}{a}}\frac{\partial}{\partial x}\sin\left(\frac{\pi x}{a}\right) = -i\hbar\sqrt{\frac{2}{a}}\left(\frac{\pi}{a}\right)\cos\left(\frac{\pi x}{a}\right)$$

Can not get definite value for momentum : $\hat{T} = \frac{\hat{p}^2}{2m} = \frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$ , $\langle \hat{Q}\rangle = \int \Psi^*\hat{Q}\Psi\,dx$

$$\langle p\rangle = \frac{2}{a}\cdot\frac{\hbar}{i}\int \sin\left(\frac{\pi x}{a}\right)\frac{\partial}{\partial x}\sin\left(\frac{\pi x}{a}\right)dx$$

$$= \frac{2\hbar}{ai}\cdot\frac{\pi}{a}\int_0^a \sin\left(\frac{\pi x}{a}\right)\cos\left(\frac{\pi x}{a}\right)dx \rightarrow = \frac{2\hbar}{ia}\int_0^0 u\,du = 0 \rightarrow p = \hbar k$$

$$\Psi(x) = \sqrt{\frac{2}{a}}\sin\left(\frac{\pi x}{a}\right) : \hat{T}\Psi = +\Psi \rightarrow -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\Psi = \frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\left(\sqrt{\frac{2}{a}}\sin\left(\frac{\pi x}{a}\right)\right)$$

$$= \frac{-\hbar^2}{2m}\cdot\sqrt{\frac{2}{a}}\cdot\frac{\pi}{a}\cdot\frac{\partial}{\partial x}\cos\left(\frac{\pi x}{a}\right) = \frac{\hbar^2}{2m}\sqrt{\frac{2}{a}}\left(\frac{\pi}{a}\right)^2\sin\left(\frac{\pi x}{a}\right) : \frac{\hbar^2}{2m}\sqrt{\frac{2}{a}}\left(\frac{\pi}{a}\right)^2\sin\left(\frac{\pi x}{a}\right)$$

$$\langle \hat{T}\rangle = \int \Psi^*\hat{T}\Psi$$

$$\langle \hat{T}\rangle = \frac{\hbar^2}{2m}\left(\frac{\pi^2}{a^2}\right)\frac{2}{a}\int_0^a \sin^2\left(\frac{\pi x}{a}\right)dx = \frac{\hbar^2}{2m}\left(\frac{\pi^2}{a^2}\right)\frac{\cancel{2}}{\cancel{a}}\cdot\frac{\cancel{a}}{\cancel{2}} = \frac{\hbar^2}{2m}\left(\frac{\pi}{a}\right)^2 : \langle \hat{T}\rangle = \frac{\hbar^2}{2m}\left(\frac{\pi}{a}\right)^2$$

$$\hat{Q} = \hat{Q}(\hat{x}, \hat{p}_x)$$

$$\hat{x} = x, \quad \hat{p} = \frac{\hbar}{i}\frac{\partial}{\partial x} = -i\hbar\frac{\partial}{\partial x}$$

$$\langle \hat{Q}\rangle = \int \Psi^*\hat{Q}\Psi\,dx, \quad \hat{T} = \frac{1}{2}m\hat{v}^2 = \frac{\hat{p}^2}{2m} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}, \quad i\hbar\frac{\partial\Psi}{\partial t} = \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \hat{u}(x)\right)\Psi$$

$$\hat{E}(t) = i\hbar\frac{\partial}{\partial x}$$

$$i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} + V\Psi, \quad \Psi(x,t) = \Psi(x)\phi(t)$$

$$i\hbar\Psi(x)\frac{\partial\phi}{\partial t} = -\frac{\hbar^2}{2m}(\phi(t))\frac{\partial^2\Psi}{\partial x^2} + V\phi(\Psi) \rightarrow i\hbar\frac{1}{\phi}\frac{\partial\phi}{\partial t} = \left(\frac{-\hbar^2}{2m}\right)\frac{1}{\Psi}\frac{\partial^2\Psi}{\partial x^2} + V'(x)$$

$$\underbrace{i\hbar \frac{1}{\phi}\frac{\partial \phi}{\partial t}} = \underbrace{\left(\frac{-\hbar^2}{2m}\right)\frac{1}{\psi}\frac{\partial^2 \psi}{\partial x^2} + V'(x)}$$

$g(t) = H(x) \longrightarrow$ Both quantities need to be constant : $[g(t) = H(x)] = E$

$$i\hbar \frac{1}{\phi(t)} \cdot \frac{\partial \phi(t)}{\partial t} = E \longleftrightarrow \frac{-\hbar^2}{2m}\cdot\frac{1}{\psi}\frac{\partial^2\psi}{\partial x^2} + (V-E) = 0 \longrightarrow -\frac{\hbar^2}{2m}\frac{\partial^2 \psi}{\partial x^2} + (V-E)\psi = 0$$

$\hookrightarrow$ Time indepent S.E.

$$\hat{H}\psi = E\psi$$

$$(\hat{T} + \hat{u})\psi = E\psi$$

$$\frac{E_n}{i\hbar} = \frac{1}{\phi}\frac{\partial \phi}{\partial t}, \quad \frac{-iE_n}{\hbar} = \frac{1}{\phi}\frac{d\phi}{dt}, \quad \frac{-iE_n}{\hbar}dt = \frac{1}{\phi}d\phi, \quad \ln(\phi) + c = \frac{-iE_n}{\hbar}t$$

$$K\phi = e^{\frac{-iE_n}{\hbar}t} \rightarrow \phi(t) \propto e^{\frac{-iE_n}{\hbar}t}$$

now :
1.) Solve TI SE
2.) Normalize
3.) Determine proper $\psi(x,0)$ from initial conditions
4.) $\psi(x,t) = \sum C_n \psi_n e^{-iE_n t/\hbar}$
$\quad = \sum C_n \phi_n(t)\psi_n(x)$

$$e^x = 1 + x + \frac{x^2}{2!} + \frac{x^3}{3!} + \ldots\ldots, \quad = \sum C_n x^n = C_0 x^0 + C_1 x^1 + C_2 x^2 + C_3 x^3 \; : \; C_0 = 1 \quad C_2 = \tfrac{1}{2} \quad C_1 = 1 \quad C_3 = \tfrac{1}{6}$$